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PUBLICATIONS OF CHURCHILL EISENHART

1934

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34-2 The Ether: Riddle of the Ages. Scientific American 151, 242-244.

1935

35-1 Solution to Problem 3652. American Mathematical Monthly 42, 118-119.

35-2 Solution to Problem E126. American Mathematical Monthly 42, 322.

35-3 A Note on "A Statistical Method for the Comparison of Heavy Mineral Suites." American Journal of Science 30, 549-553.

35-4 A Test for the Significance of Lithological Variations. Journal of Sedimentary Petrology 5, 137-145.

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36-2 Precision of Measurements (with J. L. Barnes). Handbook of Engineering Fundamentals, Ovid W. Eshbach, ed. New York: John Wiley & Sons; 2-123 through 2-128.

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40-1 On Certain Criteria for Testing the Homogeneity of Estimates of (with Frieda S. Swed). [Abstract of a paper presented at the Philadelphia meeting of the IMS, December 27, 1939.] Annals of Mathematical Statistics 11, 111-112.

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43-3 Statistical Methods and Control in Bacteriology (with P. W. Wilson). Bacteriological Reviews 7, 57-137.

43-4 Ether Versus Cyclopropane: A Statistical Comparison of Circulatory Complications After Abdominal Operations (with R. A. Simpson and N. A. Gillespie). British Journal of Anaesthesia 18, 141-159.

43-5 Measurement of the Resistance of Peas to Aphids (with R. A. Brink, C. D. Harrington, and E. M. Searles). Journal of Agricultural Research 67, 369-387.

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a. Chapter 4. Effects of Rounding or Grouping Data, 185-223.
b. Chapter 8. Planning and Interpreting Experiments for Comparing Two Standard Deviations, 267-318.
c. Chapter 14. Probability That Sample Means Are in Opposite Order to Population Means, 375-382.
d. Chapter 15. Significance of the Largest of a Set of Sample Estimates of Variance (with Herbert Solomon), 383-394.
e. Chapter 16. Inverse Sine Transformation of Proportions, 395-416.

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THE BACKGROUND AND EVOLUTION OF THE METHOD OF LEAST SQUARES

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DIGEST*

1. Introduction

The present status of the Method of Least Squares is this: Everyone uses it, but not in exactly the same way, nor for the same reasons. There is thus some similarity to the present status of Probability, with respect to which Bertrand Russell has remarked [39, p. 344]: "While interpretation in this field is controversial, the mathematical calculus itself commands the same measure of agreement as any other branch of mathematics." But the situation with respect to the Method of Least Squares is not exactly parallel: In the case of the Method of Least Squares there is complete agreement on the procedure for forming the normal equations from the fundamental observational equations; and everyone comes up with the very same numbers for the solutions of these equations, but their reasons for employing the Method of Least Squares, their understanding of its objectives and the conditions under which these are achieved, and their interpretations of end results of its application may be quite different. Furthermore, in contrast to the situation in the case of Probability, members of one "Least Squares School" are not generally aware of the existence of the others.

This somewhat extraordinary situation results from the fact that the Method of Least Squares was developed originally from three distinctly different points of view: (1) LEAST Sum of SQUARED RESIDUALS (Legendre, 1805), (2) MAXIMUM PROBABILITY of ZERO ERROR of Estimation (Gauss, 1809), and (3) LEAST Mean SQUARED ERROR of Estimation (Gauss, 1821). These differ not only in their aims and in their initial assumptions, but also in the meanings that they attach to the numbers that all three yield as a common answer to any given problem. The existence of these three different approaches to the subject, and the consequent possibility of different interpretations of the end results of applying the Method are rarely mentioned in books on the practical applications of the Method of Least Squares. The only exception of which I am aware is Whittaker and Robinson's The Calculus of Observations, first published in 1924, in chapter IX of which one finds discussions of Legendre's approach, Gauss's first approach, and Gauss's second approach, which Gauss himself definitely preferred [63, p.224]

2. Repeated Measurement of a Single Quantity and The Principle of the Arithmetic Mean

All three developments of the Method of Least Squares stemmed from

> The Principle of the Arithmetic Mean: Given a number of measurements of a single quantity, made with the same care under the same circumstances, the best value of the unknown magnitude of this quantity afforded by the measurements in hand is the arithmetic mean of their values.

The Principle of the Arithmetic Mean seems to have originated in western Europe sometime in the latter half of the 16th century A.D.; and appears to have evolved from the Method of Reversal for eliminating (or, at least, reducing) the effects of systematic errors, that is, from the technique of taking measurements in pairs such that the two members of a pair are affected by systematic errors of (approximately) equal magnitude but of opposite signs, in which case the arithmetic mean of the pair is (at least, more nearly) free from the effects of these errors. Indeed, the practice of taking several measurements of a single quantity by the same method under essentially the same circumstances--a necessary precursor to taking the arithmetic mean of such measurements--seems to have originated early in the 16th century A.D. in connection with the efforts of mariners to devise a method for determining the longitude of a ship

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at sea from observations on the deviation of a compass needle from the true north, termed the variation or declination of the needle, which had been found by Columbus and others to be northeasterly to east of the Azores, and northwesterly to the west of the Azores.1/

1/ I find that many persons today are surprised to learn that the practice of taking several measurements of a single quantity by the same method under essentially the same circumstances for the purpose of increasing one's reliance in the resulting value is a very recent development in relation to the whole history of science. In antiquity astronomy and physics were predominantly mathematical in character. The Babylonian and Greek astronomers of antiquity were primarily mathematicians; the Sun, the Moon, and the Planets were simply the objects of their mathematical analyses. Great attention was given to mathematical details; much ingenuity was shown in the solution of the mathematical problems involved; the data used to determine numerical values for the parameters in their mathematical formulae "were instances or specimens, chiefly, but not necessarily, taken from observation with all its uncertainties, not intended as important new knowledge but often simple verifications, easily accepted, of respected earlier knowledge" [76, p. 150]. At best, numerical values for parameters were determined from single observations corresponding to special or extreme circumstances that were considered to be especially favorable or decisive. The general practice was to deduce a lot from very few data. "One can ... demonstrate that [Babylonian] tables [from the period 240-40 B.C.] for the phenomena of Jupiter, computed ahead for several decades, were based on a single observational element, the rest being derived therefrom in strictly mathematical fashion. This conforms to a conscious tendency of ancient astronomers to reduce the empirical data to the barest minimum, because they were well aware of the great insecurity of direct observation." [71, p. 801] "I do not know of any case from antiquity of repeated observations of the same quantity. In principle that does not exclude that such observations were made; theoretical treatises like the Almagest [of Claudius Ptolemy, 2nd century A.D.] would not mention such things nor would they show up in computed ephemerides, etc. But I think that it is very unlikely that one ever repeated on purpose an observation in order to find a more secure value." [79]. It was the need for definitive answers to such questions as 'Was the New Star of 1572 infinitely distant from the Earth like the other stars? Or was it closer than the Moon? Or was it a comet?' that led Tycho Brahe (1546-1601) to initiate the practice of taking repeated measurements of the relative positions of heavenly bodies [76, pp. 207-208, 214].

Prior to the 17th century A.D., astronomers and physicists alike selected from the available relevant observations those that seemed to them to be the best, in the sense of being in best agreement with their own observations, accepted theory, or what seemed to be the nature of the phenomena. Claudius Ptolemy is notorious for his selection of data to suit his own ends [73]; and selection of data was the usual practice of John Flamsteed (1649-1719), the first Astronomer Royal of Great Britain, according to his official biographer, Francis Baily (1774-1844):

> "His mode of proceeding was different from that adopted at the present day. For he does not appear to have taken the mean of several observations for a more correct result. Since we find that, where more than one observation of a star has been reduced, he has generally assumed that result which seemed to him most satisfactory at the time, without any regard to the rest. Neither, in fact, did he reduce the whole (nor anything like the whole) of his observations: many days' work having been wholly omitted in his computation-book. And, moreover, many of the results, which have been actually computed in that book, have not been inserted in any of his MS catalogues; either from inadvertence, or from some suspicion of their accuracy. The reader will find many instances of this kind adduced in the Notes. So that, in fact, the British Catalogue, even corrected and enlarged as it now is, does not present a rigidly correct and faithful result of the observations; and can only be considered as an index and guide to those who may be disposed to examine more minutely the position of any particular stars, or to search into any branch of astronomy (such as the lunar or planetary motions) connected therewith. Thus, although there are 163 observations of η Geminorum, only 4 of those observations have been reduced by Flamsteed; and he has taken the result of the first reduction as the correct value. Again, there are 124 observations of γ Geminorum, yet only 2 of those have been reduced by Flamsteed; and he

has here also taken the result of the first reduction as the correct value, although there is a difference of 5' between the two. These are not singular cases, but the same method is pursued throughout the whole of his work. He seems to have been more solicitous about increasing the number of his stars in order to complete his catalogue, than anxious to reach those refinements in the art of reduction which have rendered modern observations of so much value, but which were neither known, nor even suspected, at that period." [30, p. 376. Underscoring added.]

In this connection it needs to be remembered that from the days of Pythagoras (540 ± B.C.) until Johannes Kepler (1571-1630) it was a matter of firm belief that the heavenly bodies travel in circular orbits, and when observations apparently disagreed the problem was to "save the phenomena", as it was called, by devising appropriate corrections to the observations, or by discrediting them altogether--the theory was above question! "To hold other views was not a scientific error but a heresy. Astronomy in antiquity was as thorny a subject as biblical criticism in modern times. Observational astronomy was subjected to anxious scrutiny and careful management" [82, p. 223]. Kepler, respecting this tradition, labored for nearly six years and through "at least seventy" separate calculations in his attempts to explain an 8' discrepancy in the orbit of Mars implied by Tycho Brahe's observations before recognizing, accepting, and then proving the ellipticity of its orbit.

The evolution of "taking the mean" from implicit practice to explicit principle can be summarized as follows:

1519 Before 1519, Francisco Falero, a Portuguese in the service of the Spanish Navy, and Filipe Guillen, an apothecary of Seville, had devised sun-dial instruments equipped with magnetic needles, for determining true north at sea by taking the mean of the azimuths of the gnomonic shadows corresponding to equal altitudes of the Sun before and after noon, and thence determining the declination of the magnetic needle by noting its deviation from the north so determined. [60, pp. 81-83; 64, p. 79]

535 Falero's treatise on navigation [1], published in 1535, contains the first printed description of the abovementioned technique, together with an explicit recommendation that several measurements of the magnetic declination be made on a single day in the interest of greater assurance in the value so found. [1, para 8; 64, p. 83] He says nothing on how to choose a "best value" when the values so found are nonidentical.

1538-41 Joao de Castro, utilizing a Falero-Guillen type instrument improved by the addition of a device for determining the Sun's altitude [2], recorded 43 sets of magnetic declination determinations taken on voyages from Lisbon (Portugal) to Goa (India), along the west coast of India, and in the Red Sea from India to Suez [3]. The two, three, or four values recorded (to 1/4°) for a single day are often identical, and differ at most by only 3/4°.[60, p. 85; 67, p.197]

1581 William Borough, Comptroller of the Navy of Queen Elizabeth, reports 9 values (to 1/2 min.) of the magnetic declination at Limehouse obtained by himself on October 16, 1580, using the Falero-Guillen technique and a similar instrument of his own design, "and conferring them altogether, I doe finde the true variation of the Needle on Compass at Limehouse to be about 11d. 1/4 or 11d. 1/3, which is a point of the compasso just [360°/32 = 11 1/4°] or little more" [4, chapter 3, last paragraph]. For these 9 values I find:

mean = 11° 18 8/9' = 11.32°; median = 11° 17 1/2' = 11.29°

mode = 11° 22 1/2' = 11.37°; midrange = 11° 17' = 11.28°

Clearly the operation of "conferring them altogether" is not unequivocally defined by the outcome, but I consider it reasonable to conclude that he actually took the arithmetic mean.

1602 Twenty-seven separate determinations of the right ascension of the star α Ariotis were made by the Danish nobleman, Tycho Brahe, founder of modern observational astronomy, during the period February 1582 through December 15[illegible]. To eliminate the effects of parallax and refraction, he combined 21 of these to form 12 pairs such that one determination of a pair was based on observation of Venus west of the Sun, the other on observation east of the Sun, thus

observations being so selected that the altitudes, declinations, and distances from the Earth of the Sun and Venus, respectively, were as far as possible the same in each of the two instances. From the means of these 12 pairs (whose time mid-points range from 1383 Dec. 9 to 1387 Dec. 22) and the remaining 3 individual determinations (corresponding to Feb., March, and April 1582) he adopts 26° 0' 30" as the value of the right ascension of α Arietis at the end of the year 1585, i.e. the mid-point of the period of observation, without further explanation. [5, Part 1, chapter 2, article 193; Opera, Vol. II, p. 197; 56, p. 350; 81, p. 130-132]. His data yield the following:

	12 pairs	12 pairs + 3 indiv.
mean	26° 0' 27"	26° 0' 29"
median	26° 0' 28 1/2"	26° 0 30'
mode	none	none
midrange	26° 0' 23"	26° 0' 24"
time-mean	1886 Aug. 17	1884 Sept. 26
time-midrange	1885 Dec. 2	1834 Jan. 24

Inasmuch as the coordinates of nine standard reference stars given in his star catalogue are all rounded to 5", I conclude that Tycho evaluated the midrange of the time mid-points of his 12 paired values, and the arithmetic mean of the corresponding 12 mean right ascension determinations, rounding the resulting values to the nearest half-year and nearest 5", respectively. This is certainly astute data analysis, but it is not exactly taking the arithmetic mean of several measurements of a single fixed quantity obtained by the same method under essentially the same circumstances. It exemplifies a more general technique of which taking the mean of several strictly comparable measurements is the limiting case as the range of "circumstances" involved shrinks to zero.

1622 Sometime prior to 1622, Edmund Gunter (1581-1626), Professor of Astronomy at Gresham College, London (1619-1626), worked out computational procedures for solving problems such as the following, of which he gives worked examples (among others) in his book, The Cros-staff [6]:

10. Having the Latitude of the place, and the Declination of the Sun, to find the Azimuth [of the Sun]. [10, p. 267]

13. Having the hour of the day, the Sun's Altitude, and the Declination, to find the Azimuth. [10, p. 271]

"Having these means to find the Sun's Azimuth, we may compare it with the Magnetical Azimuth, to find the variation of the Needle" [10, p. 278]. Finding in this way a "variation" of only "6 gr. 15 m.", whereas Borough had found "11 gr. 15 m." in 1580, he "enquired after the place where Mr. Borough observed, and went to Limehouse with some friends ... and towards night the 13th of June 1622" made 8 determinations of the "variation" of the Needle which he reports in full detail [10, p. 279]. The largest, "6 gr. 13m.", was more than 5° less than Borough's mean value, and nearly 5° less than Borough's smallest value, 11 gr. 11 1/2 m. Gunter seems to have regarded his data as casting doubt on the accuracy of Borough's findings, or his own; and, he does not attempt to arrive at a 'best' value for 1622 from his own data.

1635 Henry Gellibrand, Professor of Astronomy at Gresham College, London, discovers the non-constancy with respect to time of the declination of a magnetic needle at a given place, from a comparison of declination measurements made at Limehouse by William Borough in 1580, and at the same place by Edmund Gunter in 1622 and himself in 1634. Of Gunter's eight declination measurements taken on June 13, 1622 the largest was 6° 13', which was nearly 5° less than Borough's smallest value (11° 11½'), the difference being ascribed at first to errors in Borough's values. To resolve this suspicion

Gellibrand selects a particular set of Borough's shadow and needle readings corresponding to 20° 0' morning and afternoon apparent elevations of the Sun, subjects these to detailed astronomical analysis, and obtains 11° 0' 0" from the morning data and 11° 32' 28" from the afternoon data, for comparison with Borough's corresponding single declination value 11° 22' 30". The differences among these are clearly negligible. "So that if we take the Arithmeticall meane, we may probably conclude the variation [i.e. declination] answerable to his time to be about 11 gr. 16 min" [7, p. 15]. His own 11 determinations, made on June 12, 1634, ranged only from 3° 55' to 4° 12', so that "These Concordant Observations can not produce a variation greater than 4 gr. 12 min. nor less than 3 gr. 55 min., the Arithmeticall meane limiting it to 4 gr. and about 4 minutes" [7, p. 18]. The exact arithmetic mean of his values is 4° 4 9/11'.

1638 Galileo appears to have been one of the first experimental scientists to recognize the need for attaining a degree of consistency among repeated measurements of a single quantity before the method of measurement concerned can be regarded as meaningful. Thus, describing his famous experiment on the acceleration of gravity in which he allowed a ball to roll different distances down an inclined plane, Galileo wrote [8, Third Day; Nat'l. edition, p. 213]:

> "... we let, as I was saying, the ball descend through said channel, recording, in a manner presently to be described, the time it took in traversing it all, repeating the same action many times to make really sure of the magnitude of time, in which one never found a difference of even a tenth of a pulsebeat. Having done and established precisely such operation, we let the same ball descend only for the fourth part of the length of the same channel; ..."[2]

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[2] I am grateful to my colleague Ugo Fano for this translation.

1668 Vol. III of the Philosophical Transactions contains "An Extract of a Letter, written by D. B. to the Publisher" presenting a table of 5 magnetic declination measurements made near Bristol on June 13, 1666, by Capt. Samuel Sturmy, "an experienced Seaman, and a Commander of a Merchant Ship for many years," who took them "in the presence of Mr. Staynred, an ancient Mathematician, and others." "In this Table, [Capt. Sturmy] notes the greatest ... difference to be 14 minutes; and so taking the mean for the true Variation, he concludes it then and there to be just 1. deg. 27. min., viz. June 13, 1666. [9, p. 726] The exact mean of the 5 reported values is 1° 27.8'; the median=the midrange=1° 24'.

It is evident from the foregoing that taking the arithmetic mean of repeated measurements of a single quantity as the best approximation to the true value of this quantity afforded by the measurements in hand had become an established, if not universal, practice in the field of terrestrial magnetism before 1700. The practice spread to other fields, but not without some mixed cases to confuse the issue. For instance:-

1737 De Maupertuis, in his report of November 13, 1737 to the French Academy of Sciences on the measurement of a meridian arc of one degree at the Arctic Circle in Lapland, states [13, p. 422; 15, p. 36] that in measuring the angles involved "each one made his own observation and wrote it down separately, and afterwards we took the milieu [middle, or mean?] of all of these observations, which differed little from each other." The raw observations are not given here, nor in his full report [14, p. 431-466; 15, p. 79ff]. Pinkerton [83, p. 240] and Clarke [55, p. 5] translated "milieu" as "mean", and Plackett [81, p. 133] cites Clarke's rendition as unequivocal evidence of use of the arithmetic mean by de Maupertuis. Unfortunately the available evidence is mixed. In his full report, De Maupertuis gives [14, p. 435; 15, p. 36] three separate determinations of an angle PQM, namely, 28° 51' 23", 28° 51' 30", 28° 52' 22", and then says "prenant un milieu entre toutes ces declinaisons, on a pour la declination de Pullingi, ou l'angle PQM, 28° 51' 52". Here the "milieu" taken is evidently the middle in the sense of the midrange! On the other hand, later in his full report, he gives [14, p. 447; 15, p. 103] two sets of 5 measurements each

"dont le milieu" [of which the "milieu"] reported in each case is unquestionably the arithmetic mean.

In March 1755, Thomas Simpson wrote [20, p. 82-82]

> "that the method practised by astronomers, in order to diminish the errors arising from the imperfections of instruments, and of the organs of sense, by taking the Mean of several observations, has not been so generally received, but that some persons, of considerable note, have been of opinion, and even publickly maintained, that one single observation, taken with due care, was as much to be relied on as the Mean of a great number",

and then proceeded to provide a mathematical justification for practice, based on the mathematical theory of probability. More on this later. In 1757 he remarked [22, p. 64] that "the method practised by Astronomers ... [of] taking the mean of several observations, is of very great utility, and almost universally followed." Taken together these statements seem to imply that the Principle of the Arithmetic Mean had become widely, but not universally, accepted by the middle of the 18th century.

3. Measurement of Two or More Related Quantities and Minimization of Residuals

When two or more related quantities are measured individually, the resulting measured values usually fail to satisfy the constraints on their magnitudes implied by the given inter-relations among the quantities concerned. In such cases these "raw" measured values are mutually contradictory and require adjustment in order to be usable for the purpose intended. Thus, if one has an observed value for each of the three interior angles of a plane triangle, these values are strictly speaking not usable as values for those angles unless they sum to 180°. The primary goal of combination or adjustment of observations is to derive from such inconsistent measurements, if possible, adjusted values for the respective quantities concerned that do satisfy the constraints on their magnitudes imposed by the nature of the quantities themselves and by the existing interrelations among them. A second objective is to select from among all possible sets of adjusted values, a set that is "best" in some well-defined sense.

Inasmuch as the actual errors of individual observations are usually unknown and forever unknowable, attention seems to have been directed first to minimizing the apparent inconsistency of observations as evidenced by some simple function of their residuals.[a]

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[a] If $Y_1, Y_2, \ldots, Y_n$ are observed values of a magnitude α then $Y_1 - \alpha = \varepsilon_1$, $Y_2 - \alpha = \varepsilon_2, \ldots, Y_n - \alpha = \varepsilon_n$ are the errors of the respective observations. If, the value of α being unknown, one adopts some particular value for it, say a, then $Y_1 - a = R_1$, $Y_2 - a = R_2, \ldots, Y_n - a = R_n$ are the residuals of the observations corresponding to the adjusted value a.

The successive stages of this approach to the general problem of combination of observations, which culminated in Legendre's 1805 pronouncement of his version of the Method of Least Squares, were as follows:

c. 1700 When several 'equally good' measurements of a single quantity are available, the Principle of the Arithmetic Mean states that the 'best' value to take is their arithmetic mean. The arithmetic mean a of a set of measurements $Y_1, Y_2, \ldots, Y_n$ is the solution of the equation

$$\sum_1^n (Y_i - a) = 0, \tag{1}$$

that is, the value determined by the condition of zero sum of residuals. In the language of physics since the days of Archimedes (287?-212 B.C.), equation (1) says that a is the abscissa of the center of gravity of n unit masses situated ~~at abscissae $Y_1, Y_2, \ldots, Y_n$, respectively.~~

1716 Roger Cotes (1682-1716), the first Plumian Professor of Astronomy and Experimental Philosophy at Cambridge University and editor of the 2nd edition of Newton's Principia, shows in his Aestimatio errorum [11], published posthumously in 1722, how the errors of measured values of various astronomical quantities of general interest are related to the errors of the primary astronomical observations from which they are derived. For instance, on p. 21, he considers the practical problem of determining the time (of day or night) t from the observed altitude h of some star and then shows how the error dt in t resulting from an error dh in h depends functionally on h, on the observer's latitude φ, and on the angle A between the observer's meridian and the star's vertical circle. He then says [11, p. 22]:

> "In quite the same way, in other cases, one finds Limits of Error that derive their origin from the less accurate observations, because the Positions most suitable for Observing are inaccessible: so that to me hardly anything further seems to be desired once it has been shown by what argument one can obtain maximum Probability in those circumstances, where diverse observations, arranged for the same purpose, exhibit conclusions only slightly different from each other. This, however, can be done in the way of the following Example. Let p be the location of some Object as determined from a first Observation, q, r, s the locations of the same Object from subsequent Observations; let furthermore P, Q, R, S be masses inversely proportional to the lengths of the Deviations over which one can spread the Errors arising from the single Observations, and which are determined by the given Error Limits; and at the points p, q, r, s let us imagine masses P, Q, R, S and let us find their center of gravity Z: I say that the point Z is the most probable Location of the Object, which can indeed be most safely assumed to be its place."[4]

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[4] I am grateful to my colleague Franz Alt for this translation from the original Latin. William Kruskal has drawn to my attention an English translation, by Augustus De Morgan, of the portion after the first colon [84, p. 379].

We can express Cotes' proposal in terms more familiar to us today as follows. If, for example, x and y are two related variables, with $y = F(x,\beta)$, say, where β is a parameter of the relationship, so that $\beta = \varphi(x,y)$, say, and if the problem is to deduce a 'best' value for β from a number of observed values of y, say, $Y_1, Y_2, \ldots, Y_n$ corresponding to known fixed values of x, say $x_1, x_2, \ldots, x_n$, then, according to Cotes' proposal, the 'best' value to take for β is the solution $\underline{B}$ of the equation

$$\sum_{i=1}^{n} w_i(B_i - B) = 0, \tag{2}$$

namely, the weighted arithmetic mean

$$B = \frac{\sum_{i=1}^{n} w_i B_i}{\sum_{i=1}^{n} w_i} \tag{3}$$

of the individual 'observed' values

$$B_i = \varphi(x_i, Y_i), \quad (i=1,2,\ldots,n), \tag{4}$$

with weights

$$w_i = [\Delta B_i]^{-1} = \left[\left(\frac{\partial B_i}{\partial Y_i}\right) \cdot \Delta Y_i\right]^{-1}, \qquad (5)$$

$(i=1,2,\ldots,n)$, respectively, where ΔY_i is the uncertainty of Y_i, that is, the length "over which one can spread the Errors" to which Y_i is subject. This is the essence of Cotes' proposal.

Two worked examples will be helpful at this juncture:

Example 1. Suppose that $y = \beta x$, with $x, y \geq 0$, and the problem is to determine the constant of proportionality β. To this end one would ordinarily choose values $x_1, x_2, \ldots, x_n$ for x that were as large as possible, and then observe the corresponding values $Y_1, Y_2, \ldots, Y_n$ of y. If it were known that over the range of x involved the uncertainty ΔY in a measured value of Y could be considered to be (at least approximately) constant, $\Delta Y = c$, then according to Cotes' proposal the 'best' value to take for β would be the value B determined by the equation

$$\sum_{i=1}^{n}\left[\frac{c}{x_i}\right]^{-1}\left(\frac{Y_i}{x_i} - B\right) = 0, \qquad (6)$$

which may be written

$$\sum_{i=1}^{n}\left(Y_i - Bx_i\right) = 0, \qquad (7)$$

in which form it clearly expresses the condition of zero sum of residuals. The solution of (7) is

$$B = \frac{\sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} x_i} = \frac{\bar{Y}}{\bar{x}}, \qquad (8)$$

the ratio of the arithmetic means. In this case, Cotes' 'line of best fit', $y = Bx$, passes through the origin and the two-dimensional center-of-gravity of the data, $(\bar{x}, \bar{Y})$.

Example 2. Conditions and problem the same as in Example 1, except that it is known that the uncertainty ΔY_i of Y_i is directly proportional to x_i, the value of x to which it corresponds. For $\Delta Y = cx$, Cotes' procedure implies that the 'best' value to take for β is the solution of the equation

$$\sum_{i=1}^{n} c\left(\frac{Y_i}{x_i} - B\right) = 0, \qquad (9)$$

namely,

$$B = \frac{\sum_{i=1}^{n}\left(\frac{Y_i}{x_i}\right)}{n} = \overline{\left(\frac{Y}{x}\right)}, \qquad (10)$$

the arithmetic mean of the ratios.

Cotes' proposal does not generalize easily to provide a simple procedure for determining 'best' values for all of the parameters of a two- or multi-parameter relationship. The next step, therefore, was not a generalization of Cotes' procedure to multi-parameter problems, but rather an extension to multi-parameter problems of the condition of zero sum of residuals:-

1748 The requirement of zero sum of residuals alone is not sufficient to determine the 'best' values for all of the coefficients of a two- or multi-parameter line or curve from a set of observational points. Sometime before 1748 Leonhard Euler, a Swiss mathematician, physicist, and astronomer, who made extraordinary contributions to every branch of pure and applied mathematics of his time, and Tobias Mayer, a German mathematician, physicist, and astronomer, seem to have independently devised and applied [16; 17] an extension of the simple condition of zero sum of residuals that is today called the Method of Averages [62, pp. 357-363; 66, pp. 72-73]: this consists of subdividing the observational points into as many subsets as there are coefficients to be determined, the subdivision being in terms of the values of (one of) the independent variable(s), and then applying the condition of zero sum of residuals to the points of each subset.

Provided that one is thus able to form at least as many distinct observational subsets as there are unknown parameters to be determined, the Method of Averages will always come up with a value for each parameter, but there is some arbitrariness and room for subjective choice in the formation of the subsets, with consequent effect on the answers obtained. Thus, in the case of a two-parameter line $y = \alpha + \beta x$, if the x's are more or less equally spaced throughout their range, then it is customary to choose x_0 so that there are an equal number of x's greater and less than x_0; but if the number of observational points is odd, the outcome will depend on whether the middlemost point is included in the left-hand or right-hand group. If the x's are not even symmetrically dispersed within their range, then the choice of the 'best' subdivision becomes highly subjective, and the end results correspondingly "arbitrary".

1757 Sometime between 1755 and 1757, Roger Joseph Boscovich, a Dalmatian Jesuit in the service of Pope Benedict XIV who made exceptional contributions in astronomy, geodesy, physics, and mathematics [77], formulated and applied the principle that, given more than two pairs of observed values of variables x and y connected by a linear functional relationship of the form $y = \alpha + \beta x$, then the values (a and b) that one should adopt for α and β in order to obtain the line ($\bar{y} = a \mp bx$) that is most nearly in accord with all of the observations should be those determined jointly by the two conditions:--

I. The sums of the positive and negative residuals (to the y-values) shall be equal.

II. The sum of (the absolute values of) all of the residuals, positive and negative, shall be as small as possible.

Condition I states that a and b, the intercept and slope of the best fitting line $y = a + bx$, must satisfy the equation

$$\sum_{i=1}^{n} (Y_i - a - bx_i) = 0 , \tag{11}$$

which can also be written in the form

$$\bar{Y} - a - b\bar{x} = 0 . \tag{12}$$

In other words, Condition I states that the best fitting line $y = a + bx$ shall pass through the centroid $(\bar{x}, \bar{y})$ of the observational points. Condition II states that a and b must satisfy the equation

$$\sum_{i=1}^{n} |Y_i - a - bx_i| = \text{minimum} \tag{13}$$

Replacing a in equation (13) by its value

$$a = \bar{Y} - b\bar{x} \tag{14}$$

implied by equation (12), it is seen that Condition II in conjunction with Condition I requires that the slope b shall satisfy the equation

$$\sum_{i=1}^{n} |(Y_i - \bar{Y}) - b(x_i - \bar{x})| = \text{minimum} . \qquad (15)$$

Consequently, determination of the "Boscovich line" corresponding to a given set of observational points reduces to determining its slope $\underline{b}$ from equation (15) and then evaluating $\underline{a}$ from equation (14).

Boscovich seems to have evolved these criteria for determining a line of best fit to observational data sometime between 1755 and 1757. Near the end of his joint treatise with Maire [19] on determination of the Figure of the Earth from measurements of the lengths of meridian arcs and of seconds pendulums at different latitudes,[a] published in 1755, Boscovich

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[a] If the "Figure of the Earth" is an oblate ellipsoid of revolutions, and $L = L(\varphi)$ denotes the length of a meridian arc of 1° (or of a seconds pendulum) at latitude φ, then

$$L = \alpha + \beta \sin^2 \varphi,$$

neglecting higher order terms in $\sin^2 \varphi$, with

$$\frac{\beta}{\alpha} = \frac{3}{2} e^2 ,$$

$\underline{e}$ being the <u>ellipticity</u> of the ellipsoid.

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examines (pp. 499-501) the lengths of five meridian arcs measured at five different latitudes, including the arc measured by Maire and himself in the vicinity of Rome, and finds that they yield mutually inconsistent values for the ellipticity of the Earth when considered in pairs. (Several years earlier Euler [18] had noticed such mutual inconsistency of four meridian arc determinations, and disposed of the problem by applying arbitrary corrections to these determinations to make them consistent with Newton's theoretical value for the Earth's ellipticity.)

In hopes of inducing a satisfactory "best" value, he first examined the fit of the line determined by the two extreme points, i.e. the length of 1° at the equator ($\alpha = 0°$) and at the Arctic Circle ($A = 66°$). In his judgment the other three points lay farther from this line than could be accounted for by surveying errors. Next he tried the line through the equatorial point with slope equal to the arithmetic mean of the 10 individual "slopes" yielded by taking the 5 points in all possible pairs.[b] Some of the

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[b] Had he taken the weighted arithmetic means

$$B = \sum^{*} (Y_j - Y_i)(X_j - X_i) \Big/ \sum^{*} (X_j - X_i)^2 ,$$

and

$$A = \sum^{*} (Y_i x_j - Y_j x_i)(x_j - x_i) \Big/ \sum^{*} (x_j - x_i)^2$$

of the 10 individual "observed slopes"

$$b_{ij} = \begin{vmatrix} 1 & Y_i \\ 1 & Y_j \end{vmatrix} \Bigg/ \begin{vmatrix} 1 & x_i \\ 1 & x_j \end{vmatrix} , \quad (j = 1, \ldots, 4; \; j = i + 1 \ldots, 5),$$

and 10 individual "observed intercepts"

$$a_{ij} = \begin{vmatrix} Y_i & x_i \\ Y_j & x_j \end{vmatrix} \Bigg/ \begin{vmatrix} 1 & x_i \\ 1 & x_j \end{vmatrix} , \quad (i = 1, \ldots, 4; \; j = i + 1, \ldots, 5),$$

with weights $(x_j - x_i)^2$,

where

$$\sum^{*} = \sum_{i=1}^{4} \sum_{j=i+1}^{5} ,$$

he would have obtained the least squares solution in disguise [63, p. 251].

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residuals were, he felt, still too large. Noting that two of the individual "slopes" were very different from the other 8, he rejected these and tried the arithmetic mean of the eight. The resulting line now lay above all but one of the points. Discouraged, he put aside, for the time being, trying to get a 'best' value for the Earth's ellipticity from these data. [19, 497-503]. It is in Boscovich's 1757 summary [21] of this work that Boscovich states for the first time his two conditions for a line of best fit, and reports the result of analyzing the same five meridian-arc lengths by this method [21, pp. 391-392]. In this first pronouncement of his method he does not give any justification for Conditions I and II nor any indication of how he solved equation (15) to obtain the 'best' value of the slope b.

1760 In Sections 385-390 of a prose Supplement to the second volume of a three-volume treatise on Natural Philosophy in Latin hexameters by Benedict Stay [23][a],

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[a] Commenting on this treatise in 1873, Isaac Todhunter remarked [51, p. 322]: "The number of students interested both in Natural Philosophy and in Latin Verse could scarcely ever have been large; and is probably less now than formerly."

Boscovich restated his two conditions for determining the line of best fit to observational data, justifying them as follows: the first he considered to be required by the traditional assumption that positive and negative errors are of equal probability; and the second, to be necessary in order to bring the solution into closest possible agreement with the observations. He then gave a very useful algorithm of his own invention for solving equation (15) above, followed by a step-by-step illustration of its application in terms of the five meridian-arc lengths that he had considered previously. Todhunter has fittingly remarked [51, p. 332], "Boscovich's exposition of his method takes a geometrical form: it is simple, clear and instructive." A French translation of these sections is included in the Note appended to the French edition of his joint treatise with Maire [27, pp. 501-506]. His reasoning, in outline, may be found in my chapter [75, p. 202-204] in the Boscovich Memorial Volume edited by L. L. Whyte.

1783 Laplace, in his first memoir on the Figure of the Earth [32], found, like Boscovich, that the best available determinations of meridian arcs of 1° at various latitudes gave contradictory results for the ellipticity of the Earth when considered in pairs. He, therefore proposed, and carried out a test of the ellipsoidal hypothesis, that is, of whether the equation $L = a+b \sin^2 m$ is capable of representing the observed data "within the limits of the errors of observation". This test consists of fitting to these data a line of the foregoing form with a and b chosen so as to minimize the LARGEST DEVIATION, and then making a subjective judgment whether the resulting largest residual is, or is not, explainable in terms of the uncertainties of the astronomical and surveying measurements involved. After outlining a procedure for finding the line that minimizes the largest residual (which he described again in 1799 [34, Book III, Chapter 5, Section 39], and which can be read in English translation [48, pp. 417-424], Laplace applies it to his meridian arc lengths, and finds that the largest resulting residual is on the border line of acceptability, which leads him to suspect the ellipsoidal hypothesis. In this memoir he makes no attempt to deduce 'best' values for a and b, and thence of the Earth's ellipticity e (on the assumption of ellipsoidality).

1789 Laplace in his second memoir (1789) on the Figure of the Earth [33], adopted Boscovich's two criteria for a line of best fit, and gave (pp. 33-36) an algebraic formulation and derivation of Boscovich's algorithm for solving equation (15) above, with the following comments: "Boscovich has given for this purpose an ingenious method which is explained at the end of the first [French] edition of his Voyage Astronomique et Geographique [27], but as its utilization is complicated by the need to consider geometrical figures, I am going to present it here in a most simple analytical form." Laplace's algebraic formulation of Boscovich's algorithm, expressed in modern notation, is as follows:

> Consider only those terms of the summation (15) for which $x_i \neq \bar{x}$. For each such term evaluate the corresponding implied slope
>
> $$b_i = \frac{Y_i - \bar{Y}}{x_i - \bar{x}}, \quad (x_i \neq \bar{x}) . \tag{16}$$
>
> Arrange these b_i in descending order of magnitude, thus
>
> $$b_{(1)} \geq b_{(2)} \geq b_{(3)} \geq \ldots \geq b_{(m)}, \quad (m \leq n) \tag{17}$$
>
> Arrange the absolute values of their denominators in the corresponding order, thus
>
> $$|x_{(1)} - \bar{x}|, \ |x_{(2)} - \bar{x}| \ , \ldots, \ |x_{(m)} - \bar{x}| \tag{18}$$
>
> Compute the sum of all of the "absolute denominators",
>
> $$D = \sum_{j=1}^{m} |x_{(j)} - \bar{x}| . \tag{19}$$
>
> Then the sum called for in (15) will be a minimum for $b = b_{(r)}$, the rth term of the sequence (17), where r is the smallest integer for which the partial sum of the first r terms of the sequence (18) equals or exceeds one-half of the sum of the entire sequence, i.e., the smallest r for which
>
> $$\sum_{j=1}^{r} |x_{(j)} - \bar{x}| \geq \frac{1}{2} D . \tag{20}$$
>
> If in determining r the inequality sign holds, then the solution $b = b_{(r)}$ is unique; but if the equality sign holds, then the solution is not unique and (15) attains the same minimum for any value of b between $b_{(r)}$ and $b_{(r+1)}$ inclusive.

The Boscovich and Laplace algorithms for solving equation (15) are of greater generality than may seem to be the case at first sight. Their validity does not depend in any way upon the fact that the pivot point $(\bar{x}, \bar{y})$ is the centroid of the observational points (x_i, y_i). Consequently, if it is desired to determine the coefficients a and b of the line $y = a + bx$ that passes through some particular point (x_0, y_0) and satisfies Condition II, then the required value of the slope b can be found directly from either Boscovich's or Laplace's form of the algorithm, with $\bar{x}$ and $\bar{y}$ replaced by x_0 and y_0, respectively; and the corresponding value of a then found from the relation $a = y_0 - bx_0$.

1799 Laplace, in Book III, Chapter 5 of his Mecanique Celeste [31] published in 1799, discusses the Figure of the Earth in great detail. In Section 39, he describes again [48, pp. 417-424] the method that he had used in 1783 [32] to determine the line of the form $L = a+b \sin^2\varphi$ that minimizes the absolute value of the maximum residual, and then gives [48, pp. 424-434] an alternative procedure for achieving the same end "when the number of observations is

considerable". He begins Section 40 [48, pp. 434-442] with the remark: "The ellipsis, determined in the preceding article, serves to ascertain whether the elliptical figure is within the errors of observation; but it does not determine, from the measured degrees, the figure which seems most probable. It appears to me, that this last ellipsis ought to satisfy the following conditions". He then gives Boscovich's two conditions for a line of best fit--but without mention of Boscovich!--and adds: "By considering, in this manner, whole arcs, instead of degrees which have been deduced from them, we shall give to each of these degrees so much more influence, in the computation of the ellipticity of the earth, as the corresponding arc is of greater extent, which ought to be the case". To this end he extends [48, pp. 438-442] his 1789 algebraic formulation [33] of Boscovich's technique to the case of observational points of unequal weight, expressing Conditions I and II in terms of weighted residuals and appropriately modifying his own previous algebraic formulation and derivation of Boscovich's algorithm. In Section 41 [48, pp. 443-468] he utilizes data for seven meridian arcs varying in length from 1.1° to 10.7°, and in latitude from 0.0° to 73.7° first to test the ellipticity hypothesis by means of his procedure for minimization of the maximum residual, and then to determine the "most probable" value of the earth's ellipticity. To this end he applies his (second) min-max procedure to these data reduced to correspond to 1° arcs, the respective data points being taken to have equal weight, and finding the resulting minimum maximum residual of ± 48.60 double toises (i.e. 97.2 toises = 189⁺ meters) to be "exactly on the .... limit of those which might be considered as possible", he reasons that "we must therefore admit, in the elliptical hypothesis, much greater [deviations] ... therefore it seems to follow -- that the variations of the degrees of the terrestrial meridian differ sensibly from the law -- given by the hypothesis of elliptical meridians [48, p. 448]". Nevertheless, he goes on to apply his extension of the Boscovich procedure to these same data points weighted in proportion the lengths (in degrees) of the arcs actually measured, in order to find the "most probable" value of the Earth's ellipticity if it is an ellipsoid--or, more accurately, the ellipticity of the best-fitting ellipsoid--and finds that the best-fitting ellipsoid implies a residual of 86.26 double toises (i.e., 172.52 toises = 336⁺ meters) in the Lapland degree (latitude 73.7°), which "is much too great to be admitted [and thus] confirms what we have said, that the earth varies sensibly from an elliptical figure". Bowditch, however, points out here [48, p. 450] that "an error of this magnitude did--actually exist"--the length of the Lapland degree having been found to be 200 toises less on remeasurement.

1805 Adrien Marie Legendre (1752-1833), one of the outstanding French mathematicians at the end of the 18th, and start of the 19th centuries, says in the Preface to his book on "New Methods for Determining the Orbits of Comets" published in 1805 [35, p. viii]:

> "It is necessary then, when all of the conditions of the problem are expressed conveniently, to determine the coefficients in a manner that renders the errors as small as possible. For this effect, the method that appears to me the most simple and the most general consists in rendering a minimum the sum of the squares of the errors. One obtains thus as many equations as there are unknown coefficients, which serves to determine all of the elements of the orbit... the method of which I have just spoken, and which I call the Method of least squares, can be of great utility...".

An application of this procedure to the solution of three equations is given on p. 64, illustrating the now well-known rule for forming the so-called normal equations, which is stated explicitly in an Appendix "On the Method of Least Squares" [35, pp. 72-80]. (An English translation of pages 72-75, by Professors Henry A. Ruger and Helen M. Walker of Teacher's College, Columbia University, is given in David Eugene Smiths Source Book of Mathematics [61, pp. 576-579]. In this Appendix, Legendre remarks:

> "Of all the principles which can be proposed for [achieving an adjustment of observations such that] the extreme errors, positive or negative, shall be confined within as narrow limits as possible ... there is none more general, more exact, and more easy of application, than that ... which consists of rendering the sum of squares of the erros a minimum. By this

> means there is established among the errors a sort of equilibrium which, preventing the extremes from exerting an undue influence, is very well fitted to reveal that state of the system which most nearly approaches the truth."

Unfortunately, Legendre, throughout his exposition of his "Méthode des moindres quarrés", used the term "errors" for one or more accurately termed residuals. This has served to confuse the unwary and to conceal the distinction between what he merely asserted in 1805 and what Gauss in 1821 [44] showed to be a statistical property of the procedure. The essence of what he really said is this: If in the interest of achieving an objective adjustment one seeks to minimize the mutual inconsistencies of the observations as measured by some simple function of their residuals, then the practical requirements of general applicability, unique arithmetical solutions, and ease of computation lead to the adoption of the technique of Least Sum of Squared RESIDUALS. No probability considerations were involved. And his "discovery" simply marked the culmination of the attempts by Euler, Mayer, Boscovich, Laplace and others, to develop a practicable objective method of adjustment based solely on consideration of residuals.

4. Probability Distributions of Errors and "Most Probable" Values

The error of any measurement of a particular quantity is, by definition, the difference between the measurement concerned and the true value of the magnitude of this quantity, taken positive or negative according as the measurement is greater or less than the true value. In other words, if x denotes a single measurement of a quantity, or an adjusted value derived from a specific set of individual measurements, and τ is the true value of the magnitude of the quantity concerned, then, by definition,

$$\text{the error of } x \text{ as a measurement of } \tau = x - \tau$$

The error of any particular measurement, x, is, therefore, a fixed number. The numerical magnitude and sign of this number will ordinarily be unknown and unknowable, because the true value of the magnitude of the quantity concerned is ordinarily unknown and unknowable. A mathematical theory of errors is not possible so long as the errors of individual measurement are regarded as unique quantities associated with the particular measurements concerned. A mathematical theory of errors is possible only when the error of a particular measurement is regarded as instance of the errors characteristic of measurements of the same quantity that might have been, or might be, yielded by the same measurement process under the same conditions. This fundamental step was not taken until--

1755 On March 4, 1755, Thomas Simpson (1710-1761), Professor of Mathematics at the Woolwich Military Academy, addressed "A Letter to the Right Honourable George Earl of Macclesfield, President of the Royal Society, on the advantage of taking the mean of a number of observations, in practical astronomy" [20]. This remarkable letter began as follows:

> "My lord, it is well known to your Lordship, that the method practised by astronomers, in order to diminish the errors arising from the imperfections of instruments, and of the organs of sense, by taking the Mean of several observations, has not been so generally received, but that some persons, of considerable note, have been of opinion, and even publickly maintained, that one single observation, taken with due care, was as much to be relied on as the Mean of a great number.
>
> "As this appeared to me to be a matter of much importance, I had a strong inclination to try whether, by the application of mathematical principles, it might not receive some new light; from whence the utility and advantage of the method in practice might appear with a greater degree of evidence. In the prosecution of this design (the result of which I have now the honour to transmit to your Lordship) I have, indeed, been obliged to make use of an hypothesis, or to assume a series of numbers, to express the respective chances for the different errors to which any single observation is subject; ...
>
> . . . .

> "Should not the assumption, which I have made use of, appear to your Lordship so well chosen as some others might be, it will, however, be sufficient to answer the intended purpose: and your Lordship will find, on calculation that, whatever series is assumed for the chances of the happening of the different errors, the result will turn out greatly in favour of the method now practised, by taking a mean value."

Simpson's first "assumption" was that the errors of measurements of a single quantity by a particular measurement process be regarded as taking the values $-v, -v+1, \ldots, 2, 1, 0, 1, 2, \ldots, v-1, v$ with equal probabilities, i.e. a discrete uniform distribution. Second, he proposed that the errors be regarded as taking on the above values with probabilities proportional to $1, 2, \ldots, v-1, v, v+1, v, v-1, \ldots, 2, 1$, respectively, i.e. a discrete triangular distribution. Then, utilizing the generating function techniques employed extensively by Abraham De Moivre (1667-1754) and others in the solution of problems relating to tosses of dice and other games of chance, Simpson derived, for each of these assumptions, the probability distribution of the sum of n independent errors from such a distribution, and from this the corresponding distribution of the arithmetic mean of n independent errors. He summed up his findings as follows:

> "Upon the whole of which it appears, that the taking of the Mean of a number of observations, greatly diminishes the chances for all the smaller errors, and cuts off almost all possibility of any great ones: which last consideration, alone, seems sufficient to recommend the use of the method, not only to astronomers, but to all others concerned in making of experiments of any kind (to which the above reasoning is equally applicable). And the more observations or experiments there are made, the less will the conclusion be liable to err, provided they admit of being repeated under the same circumstances." [20, pp. 92-93]

It should be noted that Simpson did not prove that "taking of the arithmetic mean" was the best thing to do but merely that it is good. However, in accomplishing this goal he did something much more important: he took the bold step of regarding errors, not as individual unrelated happenings, but as properties of the measurement process itself in conjunction with the instrument employed and the observer involved. He thus opened the way to a mathematical theory of measurement based on the mathematical theory of probability.

1757 In a second paper on "the advantage of taking the mean" [22], Simpson finds the distribution of the mean of n independent errors from a continuous triangular distribution, by proceeding to the limit as the number of possible error values in the interval $(-v, +v)$ tends to infinity.

1774 Joseph Louis Lagrange (1736-1813), an Italian by birth, German by adoption and a Frenchman by choice, one of the greatest mathematicians of all time, in a long memoire "on the utility of taking the mean" [23] provides a somewhat more rigorous treatment of Simpson's analyses--without mention of Simpson--and, by similar passage to the limit, derives the distribution of the mean of n independent errors from a continuous uniform distribution. Origin of the expression "law of facility of error".

1774 Laplace in the first paper on the statistical theory of estimation [29] proposes the double-exponential distribution, $\frac{m}{2} e^{-m|y|}$, $-\infty < y < +\infty$ a law of error, where $y = x-\tau$, τ being the true value of the quantity of which x is a measurement.

1778 Daniel Bernoulli (1700-1782) proposes semi-circular law of error, $f(x) = [a^2 - y^2]^{\frac{1}{2}}$, $-a \leq y < +a$, and maximization of $\prod_{i=1}^{n} [a^2 - (x_i-\tau)^2]^{\frac{1}{2}}$ with respect to τ to obtain the "most probable" value of τ. For $n=2$ this yields $T = \bar{x}$. For $n > 3$ leads to unmanageable equations.

1773 Laplace proposes $f(x) = \frac{a}{2} \log_e\left(\frac{a}{y}\right)$, $-a < y < +a$, as a law of error.

1795-1802 In 1795, at the age of eighteen, Carl Friedrich Gauss, mathematical peer of Archimedes (287-212 B.C.) and Sir Isaac Newton (1642-1727), and unequalled in mathematical precocity, discovered the advantages of the technique of LEAST Sum of SQUARED RESIDUALS for adjustment of observations in geodesy. "Originally Gauss did not attach great importance to the method of least squares; he felt it was so natural that it must have been used by many who were engaged in numerical calculations. Frequently he said that he would be willing to bet that the elder Tobias Mayer [1723-1762] had used it in his calculations. Later he discovered by examining Mayer's papers that he would have lost the bet". [72, p. 113]. In 1797 he concluded that determination of most probable values of observed quantities required knowledge of the law of error involved [Werke, vol. IV, p. 98]. By June 1798 he had completed his now famous "first proof" via the calculus of probabilities [72, p. 113]. On January 1, 1801, Guiseppi Piazzi at Palermo discovered a new planet, Ceres, which he was able to observe only until February 11th, after which it was obscured by the Sun. His attempts to compute its orbit from so few observations were unsuccessful, and when he looked for it, when it should have emerged from the Sun's rays, he could not find it. Other European astronomers tried and also failed. The September 1801 issue of von Zach's Monatliche Correspondez gave Piazzi's complete observations, and so reached Gauss; the October issue reported that all efforts to relocate the planet had failed. Gauss's diary notes show that he was working on the Ceres problem from early November 1801 onward [72, p. 52], and before the end of 1801 Ceres was found again "at the place predicted by him" which was "quite different from the former computations" [76, p. 353]. In April 1802, Heinrich Olbers found another new planet, Pallas, in the region where he had looked for Ceres [76, p. 353]. Gauss applied his orbit calculation techniques, including the method of least squares, to evaluate the orbit of Pallas also, and then wrote up his technique and findings in a "Summary survey of the methods applied in the determination of the orbits of both new planets", which he sent to Olbers on August 6, 1802. Olbers did not return it to Gauss until November 1805 [72, p. 53], i.e., not until after the appearance of Legendre's proclamation of his own independent formulation of the "Methode des moindres quarrés" in his treatise on "New Methods for Determining the Orbits of Comets" [55]. Thus, in newspaper parlance, was Gauss scooped! Following the publication of Gauss's treatise on "Theory of the Motion of Heavenly Bodies" in 1809, in which Gauss remarked [37, Book II, Sec. 3, Article 186] that "we have made use of [this principle] since the year 1795", Legendre became indignant and accused Gauss of appropriating his method of least squares. To help set the record straight, Gauss's 1802 "Summary Survey" was published in its entirety in Zach's Monatliche Correspondez for September 1809. [38]

1808 Robert Adrian (1775-1843) of Philadelphia publishes two derivations of

$$f(y) = \frac{h}{\sqrt{\pi}} e^{-h^2y^2}, \quad -\infty < y < +\infty,$$

as a law of error, his second derivation being the two-dimensional analog (in terms of errors) of Clark Maxwell's derivation of the tri-variate normal distribution of velocities in a gas.

1809 Gauss publishes his "first proof" of the Method of Least Squares in Book II, Section 3 of his Theoria Motus [37]. In evolving his "proof" he (a) adopted as a postulate the widely accepted Principle of the Arithmetic Mean, (b) utilized the concept that repetition of a measurement process generates a probability distribution of errors, and (c) applied Bayes' method of inverse probability [25, 26] -- without reference to Bayes. Starting from these premises he showed that if the arithmetic mean of n independent measurements of a single magnitude is to be the most probable value of this magnitude a posteriori, then the errors $Y_i = x_i - \tau$ of the individual measurements x_i must be distributed in accordance with the law of error

$$f(y) = \frac{h}{\sqrt{\pi}} e^{-h^2y^2} \quad -\infty < y < +\infty.^{2/}$$

7/ Henri Poincaré (1854-1912) pointed out in 1896 [57, pp. 152-155] that Gauss's proof depends subtly on $f(y)$ being a "law of error" in the sense that the true value τ is (to use modern terminology) the scale parameter of the probability distribution of the measurement x, say,

$g(x) = \frac{h}{\sqrt{\pi}} e^{-h^2(x-\tau)^2}$. If $\bar{x}$ is merely to be the maximum likelihood estimator of some parameter θ, then a broader class of distributions is involved [57, p. 155; 68, Example 17.01].

Then he showed that, if errors are normally distributed, and if the unknown values of the essential parameters have uniform a priori distributions, then the most probable values of the unknown implied by a given set of observational data are given identically by the application of the technique of Least Sum of Squared RESIDUALS. The expression "most probable values" had, and still has, a great popular appeal; and it is this, rather than Gauss's second approach, that is usually given as "the theoretical basis" of Least Squares in traditional books on the adjustment of observations and the theory of errors. In consequence, Gauss's first "proof" of the Method of Least Squares is the best known today among applied scientists. Gauss himself, however, in a letter to Bessel (1839) rejected this justification of the Method of Least Squares on the grounds that, from a purely practical viewpoint, maximizing the probability of a zero error (of estimate) is less important than minimizing the probability of any large error (of estimate). This, his first paper on the subject remains notable, however, because in it he notes that h reflects the precision of the distribution of errors $f(y)$, and gives his famous rules for weighting results of unequal precision so as to obtain final results of maximum attainable precision.

1809 Laplace deduces [39] the Central Limit Theorem, consequently Gauss's Least Squares gives the "most probable value" under more general conditions when the number of observations is large!

5. Minimum Errors of Estimation

1774 Laplace suggests [29] that the "best mean" to take in practical astronomy is that function of the observations which has an equal probability of over- and under-estimating the true value; shows that this is equivalent to adopting the principle of Least Mean ABSOLUTE ERROR of ESTIMATION; and gives an algorithm for finding this particular function of three observations in a one-parameter case.

1778 Laplace extends the foregoing approach to the case of n independent observations in the one-parameter case [31], and terms this form of estimation the "Most Advantageous Method".

1811 Laplace shows [40] among all distributions of the form $\varphi(x) = Ke^{-\psi(x-\tau)^2}$, the normal distribution, for which $\psi(x-\tau)^2 = h^2(x-\tau)^2$, is the only one for which $\bar{x}$ is the "most advantageous" estimator of τ.

1821-23 By adopting instead the principle of Least Mean Squared ERROR of ESTIMATION and the requirement that the resulting "best mean" should yield the true values of the quantities concerned if it should happen that all of the observations were entirely free from error, Gauss shows [44, 45] that, when the resulting "best values" are linear functions of the observations, then they are identically the same as those given by the technique of Least Sum of Squared RESIDUALS, which provides the practical modus operandi for obtaining them. This fact, which mathematical statisticians today express by saying that the Method of Least Squares yields the minimum variance linear unbiased estimators of the unknown magnitudes concerned under "very general conditions", is considered by many mathematical statisticians today to be the real "theoretical basis" of the Method of Least Squares, and the explanation of the robust survival and conspicuous utility of Least Squares

as a tool of applied science. Nevertheless, this "best linear unbiased estimator" property of Least Squares seems to be unknown to many users of the Method. Moreover, this one-to-one correspondence between minimizing some function of RESIDUALS and minimizing the same function of ERRORS of ESTIMATION appears to be a unique property of least squares.

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